ASYMPTOTIC HEAT KERNEL EXPANSION IN THE SEMI-CLASSICAL LIMIT

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ABSTRACT. Let $H_\hbar = \hbar^2 L + V$ where L is a self-adjoint Laplace type operator acting on sections of a vector bundle over a compact Riemannian manifold and V is a symmetric endomorphism field. We derive an asymptotic expansion for the heat kernel of $H_\hbar$ as $\hbar \searrow 0$. As a consequence we get an asymptotic expansion for the quantum partition function and we see that it is asymptotic to the classical partition function. Moreover, we show how to bound the quantum partition function for positive $\hbar$ by the classical partition function.

1. INTRODUCTION

In this paper we study semi-classical approximations for the heat kernel of a general self-adjoint Laplace type operator in a geometric context. More precisely, let M be an n-dimensional compact Riemannian manifold without boundary and let $E \to M$ be a Riemannian or Hermitian vector bundle. Let L be a self-adjoint Laplace-type operator with smooth coefficients acting on sections of E. Important examples of such operators are the Laplace-Beltrami operator acting on functions, more generally, the Hodge-Laplacian acting on differential forms, and the square of the Dirac operator acting on spinors. We fix a symmetric endomorphism field V (the potential) which need not be a scalar multiple of the identity. For any $\hbar > 0$ we consider the self-adjoint operator $H_\hbar := \hbar^2 L + V$. One is now interested in the behavior of $H_\hbar$ as $\hbar \searrow 0$.

The solution operator $e^{-tH_\hbar}$ for the heat equation $\frac{\partial u}{\partial t} + H_\hbar u = 0$ has a smooth integral kernel $k(x, y, t, \hbar)$ which we briefly call the heat kernel. Our main result, Theorem 3.3, states that there is an asymptotic expansion

$$k(x, y, t, \hbar) \quad \overset{\hbar \searrow 0}{\sim} \quad \chi(d(x, y)) \cdot q(x, y, t\hbar^2) \cdot \sum_{j=0}^{\infty} (t\hbar^2)^j \cdot \varphi_j(x, y, t).$$

Here $d(x, y)$ denotes the Riemannian distance of x and y, χ is a suitable cut-off function, and q is explicitly given by the Euclidean heat kernel, $q(x, y, \tau) = (4\pi\tau)^{-n/2} \cdot \exp\left(-d(x, y)^2/4\tau\right)$. The φ_j are smooth sections which can be determined recursively by solving appropriate transport equations. Theorem 3.3 is optimal in the sense that the asymptotic expansion holds for all derivatives with respect to x, y, and t and is uniform in $x, y \in M$ and $t \in (0, T]$ for any $T > 0$.

Now fix $t > 0$ and define the quantum partition function $Z_Q(\hbar) := \mathrm{Tr}(e^{-tH_\hbar})$. As a direct consequence of Theorem 3.3 we get Corollary 4.1

$$Z_Q(\hbar) \quad \overset{\hbar \searrow 0}{\sim} \quad (2\sqrt{\pi t}\hbar)^{-n} \cdot \sum_{j=0}^{\infty} a_j(t) \cdot (t\hbar^2)^j \tag{1}$$

This result has been proved in [10, Sec. 2] by technically rather involved methods from pseudo-differential calculus. The corresponding classical partition function is given by $Z_C(\hbar) = (2\pi\hbar)^{-n} \int_{T^*M} \mathrm{tr} \left(\exp(-t(|p|^2 \cdot \mathrm{id} + V(x))) \right) dp dx$. We directly obtain Corollary 4.2:

$$\lim_{\hbar \searrow 0} \frac{Z_Q(\hbar)}{Z_C(\hbar)} = 1. \tag{2}$$

This asymptotic statement corresponds to the following bound valid for small positive $\hbar$ (Corollary 4.7):

$$\frac{Z_Q(\hbar)}{Z_C(\hbar)} \ \leq \ c_3 \cdot e^{c_2 \cdot t\hbar^2} \cdot \frac{v_{0,n}\left(\sqrt{t\hbar^2}\right)}{v_{K,n}\left(\sqrt{t\hbar^2}\right)}.$$

Here $v_{K,n}(r)$ denotes the volume of the geodesic ball of radius r in the n-dimensional model space of constant curvature K. The constant c_3 depends only on the dimension n of M, the constant c_2 depends on n, on a lower bound for the Ricci curvature, and on a lower bound for the potential of L.

In the case that the underlying manifold is Euclidean space and the operator L is the classical Laplace operator acting on functions the optimal inequality

$$\frac{Z_Q(\hbar)}{Z_C(\hbar)} \ \leq \ 1$$

was independently obtained by Golden [5], Symanzik [14], and Thompson [15]. In this classical situation (2) can be found in Simon's book [13, Thm. 10.1]. In the case of a general compact manifold the asymptotic expansion of $Z_Q(\hbar)$ is contained in [10, Prop. 2.4].

Our methods are rather direct and explicit. We use standard facts from geometric analysis. The estimates on the quantum partition function are based on the Golden-Thompson inequality, the Hess-Schrader-Uhlenbrock estimate and an estimate on the heat kernel of the Laplace-Beltrami operator due to Schoen and Yau. No pseudo-differential calculus or microlocal analysis are needed.

2. THE HEAT KERNEL

Let M be an n-dimensional compact Riemannian manifold without boundary. In local coordinates the Riemannian metric is denoted by g_{ij}, its inverse matrix by g^{ij}.

Let $E \to M$ be a Riemannian or Hermitian vector bundle. We denote the metric on E by $\langle \cdot, \cdot \rangle$. Let L be a self-adjoint Laplace-type operator with smooth coefficients

acting on sections of E. In local coordinates $x = (x^1, \ldots, x^n)$ and with respect to a local trivialization of E we have

$$L = -g^{ij}(x)\partial_i\partial_j + b^k(x)\partial_k + c(x).$$

Here the Einstein summation convention is understood, $b^k(x)$ and $c(x)$ are matrices depending smoothly on x, and $\partial_i = \frac{\partial}{\partial x^i}$.

It is well-known [1, Prop. 2.5] that L can globally be written in the form

$$L = \nabla^*\nabla + W$$

where ∇ is a metric connection on E, ∇^* is its formal L^2-adjoint, and W is a smooth section of $\mathrm{Sym}(E)$, the bundle of fiberwise symmetric endomorphisms of E.

Example 2.1. Let E be the trivial line bundle, i. e. sections of E are nothing but functions. Let the connection be the usual derivative, $\nabla = d$, and let $W = 0$. Then $L = \Delta = d^*d = -\mathrm{div} \circ \mathrm{grad}$, the Laplace-Beltrami operator.

Example 2.2. More generally, let $E = \Lambda^p T^*M$ be the bundle of p-forms. Then the Hodge-Laplacian $L = d^*d + dd^*$ is a self-adjoint Laplace-type operator. Here ∇ is the connection induced on E by the Levi-Civita connection. For example, for $p = 1$, the *Bochner formula* says $L = \nabla^*\nabla + \mathrm{Ric}$, see [2, p. 74, formula (2.51)] or [7, Chap. 2, Cor. 8.3].

Example 2.3. Let M carry a spin structure and let E be the spinor bundle. If D is the Dirac operator, then by the *Lichnerowicz-Schrödinger formula* $L := D^2 = \nabla^*\nabla + \frac{1}{4}\mathrm{scal}$, see [9] or [7, Chap. 2, Thm. 8.8].

Now fix another section $V \in C^\infty(M, \mathrm{Sym}(E))$. For $\hbar > 0$ we define the self-adjoint operator

$$H_\hbar := \hbar^2 L + V. \tag{3}$$

For $t > 0$ we use functional calculus to define the operator $e^{-tH_\hbar}$ as a bounded self-adjoint operator on the Hilbert space of square integrable sections of E, $L^2(M, E)$. For any $u_0 \in L^2(M, E)$ we can put $u(x, t) := (e^{-tH_\hbar}u_0)(x)$ and we get the unique solution to the heat equation

$$\frac{\partial u}{\partial t} + H_\hbar u = 0$$

subject to the initial condition

$$u(x, 0) = u_0(x).$$

By elliptic theory $e^{-tH_\hbar}$ is smoothing and its Schwartz kernel $k(x, y, t, \hbar)$ depends smoothly on all variables $x, y \in M$, $t, \hbar > 0$, see [1, Sec. 2.7].

By $E \boxtimes E^* \to M \times M$ we denote the exterior tensor product bundle of E with its dual bundle E^*. Its fiber over $(x, y) \in M \times M$ is given by $(E \boxtimes E^*)_{(x,y)} = E_x \otimes E_y^* = \mathrm{Hom}(E_y, E_x)$. Note that for fixed t and $\hbar$ the heat kernel $k(\cdot, \cdot, t, \hbar)$ is a section of $E \boxtimes E^*$. We define

$$q : M \times M \times (0, \infty) \to \mathbb{R}, \qquad q(x, y, t) := (4\pi t)^{-n/2} \cdot \exp\left(-\frac{d(x, y)^2}{4t}\right),$$

where $d(x, y)$ denotes the Riemannian distance of x and y. For technical reasons we define

$$M \bowtie M := M \times M \setminus \{(x, y) \mid x \text{ and } y \text{ are cut-points}\}.$$

Recall that x and y are cut-points if either there are several geodesics of minimal length joing x and y or there is a Jacobi field along the unique shortest geodesic which vanishes at x and y. For example, on the standard sphere cut points are exactly antipodal points. One always has that $M \bowtie M$ contains the diagonal and is an open dense subset of $M \times M$. The function q is smooth on $M \bowtie M \times (0, \infty)$. We will often abbreviate $r := d(x, y)$. Then r^2 is a smooth function on $M \bowtie M$ and r itself is smooth on $M \bowtie M$ away from the diagonal.

By grad_x we denote the gradient with respect to the variable x, similarly for Δ_x, $H_{\hbar, x}$, and ∇_x. Straightforward computation yields

$$\mathrm{grad}_x q \;=\; -\frac{q}{4t}\mathrm{grad}_x(r^2) \tag{4}$$

$$\Delta_x q \;=\; -q \cdot \left(\frac{r^2}{4t^2} + \frac{\Delta_x(r^2)}{4t}\right) \tag{5}$$

$$\frac{\partial q}{\partial t} \;=\; q \cdot \left(\frac{r^2}{4t^2} - \frac{n}{2t}\right) \tag{6}$$

$$\left(\frac{\partial}{\partial t} + \Delta_x\right) q \;=\; -q \cdot \frac{2n + \Delta_x(r^2)}{4t} \tag{7}$$

3. The formal heat kernel

Now we make the following ansatz for a formal heat kernel of $H_\hbar$ over $M \bowtie M$:

$$\hat{k}(x, y, t, \hbar) = q(x, y, t\hbar^2) \cdot \sum_{j=0}^{\infty} (t\hbar^2)^j \cdot \varphi_j(x, y, t). \tag{8}$$

Lemma 3.1. *There are unique continuous sections φ_j over $M \bowtie M \times [0, \infty)$, smooth over $M \bowtie M \times (0, \infty)$, such that*

   (i) $\varphi_0(y, y, 0) = \mathrm{id}_{E_y}$ *for all $y \in M$,*

   (ii) $\left(\frac{\partial}{\partial t} + H_{\hbar, x}\right) \hat{k} = 0.$

Assertion (i) means that for fixed y and $\hbar$ any partial sum of the formal heat kernel $\hat{k}$ converges to the delta function at y since this is clearly the case for q. Assertion (ii) is to be understood in the sense that the formal series in the definiton (8) of $\hat{k}$ is differentiated termwise and then regrouped by powers of $\hbar$.

Proof of Lemma 3.1. Using (4), (7), and $\nabla^*\nabla(f\varphi) = \Delta(f)\varphi - 2\nabla_{\mathrm{grad}f}\varphi + f\nabla^*\nabla\varphi$ we compute

$$\left(\frac{\partial}{\partial t} + H_{\hbar, x}\right)\hat{k}$$

$$= \sum_{j=0}^{\infty} \left\{ \left(\frac{\partial}{\partial t} + \hbar^2\Delta_x\right)(q(x, y, t\hbar^2)) \cdot (t\hbar^2)^j \cdot \varphi_j + q \cdot \frac{\partial}{\partial t}((t\hbar^2)^j \cdot \varphi_j) \right.$$

$$\left. -2\hbar^2 \cdot (t\hbar^2)^j \cdot \nabla_{\mathrm{grad}_x q}\varphi_j + q \cdot (t\hbar^2)^j \cdot H_{\hbar, x}\varphi_j \right\}$$

$$= q \cdot \sum_{j=0}^{\infty} (t\hbar^2)^j \left\{ -\hbar^2\frac{2n + \Delta_x(r^2)}{4t\hbar^2}\varphi_j + \frac{j}{t}\varphi_j + \frac{\partial}{\partial t}\varphi_j \right.$$

$$\left. -2\hbar^2\nabla_{\frac{-1}{4t\hbar^2}\mathrm{grad}_x(r^2)}\varphi_j + \hbar^2 L_x\varphi_j + V\varphi_j \right\}$$

$$
\begin{aligned}
= \quad & q \cdot \sum_{j=0}^{\infty} t^{j-1} \hbar^{2j} \Bigg\{ -\frac{2n + \Delta_x(r^2)}{4} \varphi_j + j\varphi_j + t\frac{\partial}{\partial t}\varphi_j \\
& \quad + \nabla_{\frac{1}{2}\mathrm{grad}_x(r^2)} \varphi_j + \hbar^2 t L_x \varphi_j + tV\varphi_j \Bigg\} \\
= \quad & q \cdot \sum_{j=0}^{\infty} t^{j-1} \hbar^{2j} \Bigg\{ \left(j - \frac{2n + \Delta_x(r^2)}{4} + tV \right) \varphi_j + t\frac{\partial}{\partial t}\varphi_j \\
& \quad + r\nabla_{\mathrm{grad}_x(r)} \varphi_j + L_x \varphi_{j-1} \Bigg\}.
\end{aligned}
$$

Thus assertion (ii) is equivalent to the recursive *transport equations*

$$
t\frac{\partial}{\partial t}\varphi_j + r\nabla_{\mathrm{grad}_x(r)}\varphi_j + \left(j - \frac{2n + \Delta_x(r^2)}{4} + tV \right) \varphi_j = -L_x\varphi_{j-1} \quad (9)
$$

for $j = 0, 1, \ldots$ where we use the convention $\varphi_{-1} \equiv 0$. The function $G :=$ $(2n + \Delta_x(r^2))/4$ appearing in (9) is smooth on $M \bowtie M$ and vanishes on the diagonal $\{r = 0\}$.

We observe that the transport equation (9) is an ordinary differential equation along the integral curves of the vector field $t\frac{\partial}{\partial t} + r\frac{\partial}{\partial r}$ in the r-t-surface, see Fig. 1. More precisely, if we fix an angle θ and put $t = \cos(\theta) \cdot s$ and $r = \sin(\theta) \cdot s$, then (9) translates into

$$
s\frac{\partial}{\partial s}\varphi_j + (j - G + \cos(\theta)sV)\,\varphi_j = -L_x\varphi_{j-1} \quad (10)
$$

Here we identify the fibers of E by parallel transport along the radial geodesics γ emanating from y so that $r\nabla_{\mathrm{grad}_x(r)}$ becomes identified with $r\frac{\partial}{\partial r}$.
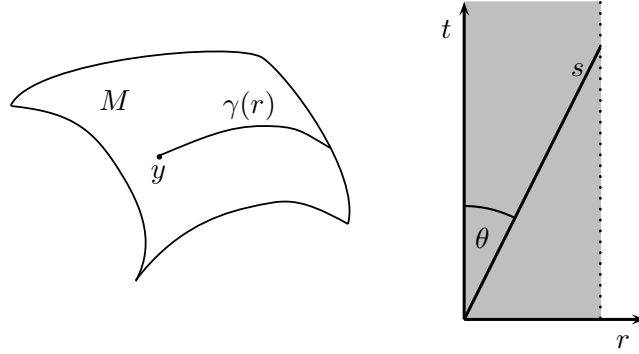

Fig. 1. Various parameters and their relation

Since this differential equation is singular at $s = 0$ we need to introduce integrating factors. In order to write them down we solve the linear ODE

$$
\frac{d}{ds}A(s) = A(s) \cdot \cos(\theta) \cdot V(\gamma(\sin(\theta)s)), \qquad A(0) = \mathrm{id}, \quad (11)
$$

in the space of endomorphisms of E_y. Of course, A depends smoothly on all data such as s, θ, $y = \gamma(0)$, and $\dot{\gamma}(0)$. As long as $A(s)$ is regular the determinant of $A(s)$ satisfies the linear ODE

$$
\frac{d}{ds}\det(A(s)) = \det(A(s)) \cdot \cos(\theta) \cdot \mathrm{tr}(V(\gamma(\sin(\theta)s))),
$$

hence $\det(A(s))$ cannot vanish anywhere since it would otherwise have to be identically 0 contradicting the initial condition $\det(A(0)) = 1$. Thus $A(s)$ remains invertible for all s. We now define

$$R_j(s) := s^j \cdot \exp\left(-\int_0^s \frac{G\,d\sigma}{\sigma}\right) \cdot A(s).$$

Since G is smooth and vanishes at $s = 0$ the integrand G/σ is smooth along the segment parametrized by $[0, s]$. Direct computation shows that (10) is equivalent to

$$\frac{\partial}{\partial s}(R_j\varphi_j) = -s^{-1}R_jL_x\varphi_{j-1} \tag{12}$$

For $j = 0$ this means that $R_0\varphi_0 = C_0$ is constant, i. e. $\varphi_0 = C_0 \cdot R_0^{-1} = C_0 \cdot \exp\left(\int_0^s \frac{G\,d\sigma}{\sigma}\right) \cdot A(s)^{-1}$. The initial condition (i) is now equivalent to $C_0 = 1$. Thus we have

$$\varphi_0 = \exp\left(\int_0^s \frac{G\,d\sigma}{\sigma}\right) \cdot A(s)^{-1}. \tag{13}$$

For $j \geq 1$ we note that $s^{-1}R_j$ is smooth also at $s = 0$ and we get $R_j\varphi_j = -\int_0^s \sigma^{-1}R_jL_x\varphi_{j-1}d\sigma + C_j$. Evaluation at $s = 0$ shows $C_j = 0$. We therefore have

$$\varphi_j = -R_j^{-1}\int_0^s \sigma^{-1}R_jL_x\varphi_{j-1}d\sigma.$$

We have established uniqueness of the φ_j. As to existence we only need to ensure that (13) and (3) define *smooth* sections over $M \bowtie M \times (0,\infty)$. For $(x,y) \in M \bowtie M$ and $r \in [0,1]$ we let $\overline{xy} : [0,1] \to M$ be the unique shortest geodesic with $\overline{xy}(0) = y$ and $\overline{xy}(1) = x$. In other words, in terms of the Riemannian exponential map $\overline{xy}(r) = \exp_y(r\exp_y^{-1}(x))$. The map $M \bowtie M \times [0,1] \to M$, $(x,y,r) \mapsto \overline{xy}(r)$, is smooth. Substituting $\sigma = us$ equation (13) can be rewritten as

$$\varphi_0(x,y,t) \;=\; \exp\left(\int_0^1 u^{-1}G(\overline{xy}(u),y)\,du\right) \cdot A(\sqrt{d(x,y)^2 + t^2})^{-1} \tag{14}$$

and (3) becomes

$$\varphi_j(x,y,t)$$
$$= \; -R_j(x,y,t)^{-1}\int_0^1 u^{-1}R_j(\overline{xy}(u),y,ut)\cdot(L_x\varphi_{j-1})(\overline{xy}(u),y,ut)du$$

where

$$R_j(x,y,t)$$
$$= \; (d(x,y)^2 + t^2)^{j/2}\cdot\exp\left(-\int_0^1 \frac{G(\overline{xy}(u),y)\,du}{u}\right)\cdot A(\sqrt{d(x,y)^2 + t^2}).$$

This shows smoothness of the φ_j on $M \bowtie M \times (0,\infty)$ and continuity on $M \bowtie M \times [0,\infty)$. $\qquad\square$

Remark 3.2. If $\theta = 0$, i.e., if $s = t$ and $x = y$, then (11) becomes a linear ODE with constant coefficients,

$$\frac{d}{ds}A(s) = A(s)\cdot V(y), \qquad A(0) = \mathrm{id},$$

and can be solved explicitly,

$$A(s) = \exp(sV(y)).$$

In particular, since $G(\overline{yy}(u), y) = G(y, y) = 0$, (14) becomes

$$\varphi_0(y, y, t) = \exp(-tV(y)) \tag{15}$$

Construction of the approximate kernel. Now we fix $\eta > 0$ smaller than the injectivity radius of M. This means that $\{r \le \eta\} \subset M \bowtie M$. We choose a smooth cutoff function $\chi : \mathbb{R} \to \mathbb{R}$ such that $\chi \equiv 1$ on $(-\infty, \eta/2]$ and $\chi \equiv 0$ on $[\eta, \infty)$. For $N \in \mathbb{N}$ we set

$$\hat{k}^{(N)}(x, y, t, \hbar) := \chi(d(x, y)) \cdot q(x, y, t\hbar^2) \cdot \sum_{j=0}^{N} (t\hbar^2)^j \cdot \varphi_j(x, y, t). \tag{16}$$

Note that $\hat{k}^{(N)}$ is a smooth section of $E \boxtimes E^*$ over $M \times M \times (0, \infty) \times (0, \infty)$ and not just over $M \bowtie M \times (0, \infty) \times (0, \infty)$.

Theorem 3.3. *Let M be an n-dimensional compact Riemannian manifold without boundary. Let $E \to M$ be a Riemannian or Hermitian vector bundle and let $H_\hbar$ be as in (3). Let $k(x, y, t, \hbar)$ be the heat kernel of $H_\hbar$.*
Let $T > 0$ and $\ell, j \in \mathbb{N}_0$. For $N > n + \ell + j$ let $\hat{k}^{(N)}(x, y, t, \hbar)$ be the approximate heat kernel as defined in (16). Then

$$\sup_{t \in (0, T]} \left\| \frac{\partial^j}{\partial t^j} \left(k - \hat{k}^{(N)} \right) \right\|_{C^\ell(M \times M)} = O(\hbar^{2N+1-2n-2\ell-2j}) \qquad (\hbar \searrow 0).$$

Proof. By construction of $\hat{k}^{(N)}$ we have (using that $q = O((t\hbar^2)^{-n/2})$ and $q = O((t\hbar^2)^\infty)$ in the region where $\chi(d(x, y))$ is not locally constant):

$$
\begin{aligned}
r_N &:= \left(\frac{\partial}{\partial t} + H_{\hbar,x} \right) (\hat{k}^{(N)} - k) \\
&= \left(\frac{\partial}{\partial t} + H_{\hbar,x} \right) (\hat{k}^{(N)}) \\
&= \chi(d(x, y)) \cdot \left(\frac{\partial}{\partial t} + H_{\hbar,x} \right) \left(q \cdot \sum_{j=0}^{N} (t\hbar^2)^j \cdot \varphi_j \right) + O((t\hbar^2)^\infty) \\
&= \chi(d(x, y)) \cdot q \cdot t^N \hbar^{2N+2} L_x \varphi_N + O((t\hbar^2)^\infty) \\
&= O(t^{N-n/2} \hbar^{2N+2-n}).
\end{aligned}
$$

Similarly, for any $m \in \mathbb{N}$ we get

$$(H_{\hbar,x})^m (r_N) = O(t^{N-n/2-2m} \hbar^{2N+2-n-2m})$$

and

$$(L_y)^m (r_N) = O(t^{N-n/2-2m} \hbar^{2N+2-n-4m}).$$

By the choice of the initial condition $\hat{k}^{(N)} - k$ vanishes at $t = 0$. Thus uniqueness of the solution to the heat equation (Duhamel's principle) implies

$$(\hat{k}^{(N)} - k)(x, y, t, \hbar) = \int_0^t e^{-(t-s)H_{\hbar,x}} r_N(\cdot, y, s, \hbar) ds.$$

The spectrum of L is bounded from below, hence $H_\hbar = \hbar^2 L + V \geq -c_1$ for all $\hbar \leq 1$ where c_1 is a suitable positive constant. Thus we have for the L^2-L^2-operator norm

$$\|e^{-(t-s)H_{\hbar,x}}\|_{L^2,L^2} \quad \leq \quad e^{c_1 t}.$$

Therefore we get for all $t \in (0, T]$

$$
\begin{aligned}
\|(\hat{k}^{(N)} - k)(\cdot, y, t, \hbar)\|_{L^2(M)} &\leq \int_0^t \|e^{-(t-s)H_{\hbar,x}}\|_{L^2,L^2} \cdot \|r_N(\cdot, y, s, \hbar)\|_{L^2(M)} ds \\
&\leq \int_0^t e^{c_1 t} \cdot c_2 \cdot s^{N-n/2} \hbar^{2N+2-n} ds \\
&\leq c_3(T) \cdot \hbar^{2N+2-n}.
\end{aligned}
$$

Furthermore,

$$
\begin{aligned}
&\|L_x(\hat{k}^{(N)} - k)(\cdot, y, t, \hbar)\|_{L^2(M)} \\
&= \hbar^{-2}\|(H_{\hbar,x} - V))(\hat{k}^{(N)} - k)(\cdot, y, t, \hbar)\|_{L^2(M)} \\
&\leq \hbar^{-2}\left\|H_{\hbar,x} \int_0^t e^{-(t-s)H_{\hbar,x}} r_N(\cdot, y, s, \hbar) ds\right\|_{L^2(M)} \\
&\quad + c_4 \hbar^{-2}\|(\hat{k}^{(N)} - k)(\cdot, y, t, \hbar)\|_{L^2(M)} \\
&\leq \hbar^{-2}\left\|\int_0^t e^{-(t-s)H_{\hbar,x}} H_{\hbar,x} r_N(\cdot, y, s, \hbar) ds\right\|_{L^2(M)} + O_T(\hbar^{2N-n}) \\
&\leq \hbar^{-2} \cdot c_5(T) \cdot \|H_{\hbar,x} r_N(\cdot, y, s, \hbar)\|_{L^2(M)} + O_T(\hbar^{2N-n}) \\
&= O_T(\hbar^{2N-n-2})
\end{aligned}
$$

and

$$
\begin{aligned}
\|L_y(\hat{k}^{(N)} - k)(\cdot, y, t, \hbar)\|_{L^2(M)} &= \left\|\int_0^t e^{-(t-s)H_{\hbar,x}} L_y r_N(\cdot, y, s, \hbar) ds\right\|_{L^2(M)} \\
&= O_T(\hbar^{2N-2-n}).
\end{aligned}
$$

Here the lower index T in $O_T(\cdots)$ indicates that the constant bounding the $O_T(\hbar^{2N-n-2})$-term by $\hbar^{2N-n-2}$ depends on T. Integration with respect to y yields

$$\|(L_x + L_y)(\hat{k}^{(N)} - k)(\cdot, \cdot, t, \hbar)\|_{L^2(M \times M)} = O_T(\hbar^{2N-2-n}).$$

Inductively, we get

$$\|(L_x + L_y)^m(\hat{k}^{(N)} - k)(\cdot, \cdot, t, \hbar)\|_{L^2(M \times M)} = O_T(\hbar^{2N+2-n-4m}).$$

By the elliptic estimates we have for the Sobolev norms

$$\|(\hat{k}^{(N)} - k)(\cdot, \cdot, t, \hbar)\|_{H^{2m}(M \times M)} = O_T(\hbar^{2N+2-n-4m})$$

and by the Sobolev embedding theorem

$$\|(\hat{k}^{(N)} - k)(\cdot, \cdot, t, \hbar)\|_{C^\ell(M \times M)} = O_T(\hbar^{2N+1-2n-2\ell}).$$

Similarly, we have

$$\|r_N(\cdot, \cdot, t, \hbar)\|_{C^\ell(M \times M)} = O_T(\hbar^{2N+1-2n-2\ell}).$$

It remains to control the t-derivatives. We compute

$$
\begin{aligned}
\frac{\partial}{\partial t}(\hat{k}^{(N)} - k) &= -H_{\hbar,x}(\hat{k}^{(N)} - k) + r_N \\
&= -\hbar^2 L_x(\hat{k}^{(N)} - k) - V \cdot (\hat{k}^{(N)} - k) + r_N,
\end{aligned}
$$

thus

$$
\begin{aligned}
&\left\| \frac{\partial}{\partial t}(\hat{k}^{(N)} - k) \right\|_{C^\ell(M \times M)} \\
&\leq \quad \hbar^2 \cdot c_6 \cdot \| \hat{k}^{(N)} - k \|_{C^{\ell+2}(M \times M)} + c_7 \cdot \| \hat{k}^{(N)} - k \|_{C^\ell(M \times M)} \\
&\quad + \| r_N \|_{C^\ell(M \times M)} \\
&= \quad \mathrm{O}_T(\hbar^{2N+1-2n-2\ell-2}).
\end{aligned}
$$

An induction finally proves the theorem. $\qquad\square$

Remark 3.4. We were somewhat generous in the application of the Sobolev embedding theorem. With a little more care we can improve the statement of Theorem 3.3 as follows:
If in addition to T, ℓ, j and N we are given $\varepsilon > 0$, then

$$
\sup_{t \in (0,T]} \left\| \frac{\partial^j}{\partial t^j} \left(k - \hat{k}^{(N)} \right) \right\|_{C^\ell(M \times M)} = \mathrm{O}(\hbar^{2N+2-\varepsilon-2n-2\ell-2j}) \qquad (\hbar \searrow 0).
$$

Remark 3.5. It would be nice to extend Theorem 3.3 to operator families of the form

$$
H_\hbar = \hbar^2 L + \hbar D + V
$$

where D is a formally self-adjoint differential operator of first order. However, this seems not to work. The resulting transport equations can no longer be solved.
There is a different approximation in [10] working also for $D \neq 0$. It is less explicit and makes heavy use of asymptotic expansions of total symbols of pseudodifferential operators. For the trace of the heat operator it seems to give the same result. We discuss this in the next section.

4. The classical and quantum partition functions

Applying Theorem 3.3 with $j = \ell = 0$ we have in particular

$$
|k(x, y, t, \hbar) - \hat{k}^{(N)}(x, y, t, \hbar)| \quad \leq \quad C \cdot \hbar^{2N+1-2n}
$$

for all $t \in (0, T]$, $x, y \in M$, and for $\hbar \searrow 0$. We put $x = y$, take the pointwise trace and integrate over M to obtain

Corollary 4.1. *Let M be an n-dimensional compact Riemannian manifold without boundary. Let $E \to M$ be a Riemannian or Hermitian vector bundle and let $H_\hbar$ be as in (3). Let $T > 0$. Then we have an asymptotic expansion*

$$
\mathrm{Tr}(e^{-tH_\hbar}) \quad \sim \quad (2\sqrt{\pi t}\hbar)^{-n} \cdot \sum_{j=0}^{\infty} a_j(t) t^j \cdot \hbar^{2j} \qquad (\hbar \searrow 0)
$$

uniform in $t \in (0, T]$.

Proof. This follows directly from Theorem 3.3 together with $q(y, y, t\hbar^2) = (4\pi t\hbar^2)^{-n/2}$ and $a_j(t) = \int_M \mathrm{tr}(\varphi_j(y, y, t)) \, dy$. $\qquad\square$

We fix $t > 0$ and we define the *quantum partition function*

$$Z_Q(\hbar) := \text{Tr}(e^{-tH_\hbar}) \tag{17}$$

and the corresponding classical quantity

$$Z_C(\hbar) := (2\pi\hbar)^{-n} \int_{T^*M} \text{tr}\left(\exp(-t(|p|^2 \cdot \text{id} + V(x)))\right) \, dpdx. \tag{18}$$

If E is the trivial line bundle and V is the potential energy this is the partition function in statistical mechanics with $t = 1/k_B T$ where T is the temperature and k_B is Boltzmann's constant. For convenience, we call it the *classical partition function* also in our more general situation. Then we have

Corollary 4.2. *Let M be an n-dimensional compact Riemannian manifold without boundary. Let $Z_Q(\hbar)$ and $Z_C(\hbar)$ be defined as in (17) and (18). Then*

$$\lim_{\hbar \searrow 0} \frac{Z_Q(\hbar)}{Z_C(\hbar)} = 1.$$

Proof. Using $\int_{\mathbb{R}^n} \exp(-t|p|^2) \, dp = (\pi/t)^{n/2}$ and (15) we get

$$
\begin{aligned}
Z_C(\hbar) &= (2\pi\hbar)^{-n} \cdot \int_{T^*M} \text{tr}\left(\exp(-t|p|^2)\exp(-t \cdot V(x))\right) \, dpdx \\
&= (2\pi\hbar)^{-n} \cdot (\pi/t)^{n/2} \cdot \int_M \text{tr}(\exp(-t \cdot V(x))) \, dx \\
&= (2\sqrt{\pi t}\hbar)^{-n} \cdot \int_M \text{tr}(\varphi_0(x,x,t)) \, dx \\
&= (2\sqrt{\pi t}\hbar)^{-n} \cdot a_0(t).
\end{aligned}
$$

The assertion follows from Corollary 4.1. $\qquad\square$

In the remainder of this section we will contrast this asymptotic comparison of $Z_Q(\hbar)$ and $Z_C(\hbar)$ with an inequality of the two partition functions which works for positive $\hbar$. For this we need the following version of the Golden-Thompson inequality (see [4], [8] or [12]).

Lemma 4.3. *Let B and C be self-adjoint operators on a Hilbert space H, both bounded from below and such that $B + C$ is essentially self-adjoint on the intersection $\text{dom}(B) \cap \text{dom}(C)$ of the domains of B and C. Then*

$$\text{Tr}\left(\exp(-(B+C))\right) \leq \text{Tr}\left(\exp(-B)\exp(-C)\right).$$

We will also need the following elementary assertion.

Lemma 4.4. *Let A_1 and A_2 be complex $N \times N$-matrices. Let A_2 be Hermitian and nonnegative. Then*

$$|\text{tr}\left(A_1 A_2\right)| \leq |A_1| \cdot \text{tr}\left(A_2\right) \tag{19}$$

where $|A_1|$ denotes the operator norm of A_1.

Proof. Since A_2 is Hermitian and nonnegative there is a nonnegative Hermitian matrix B such that $A_2 = B^2$. For the standard basis $e_1, \ldots, e_N$ of $\mathbb{C}^N$ and the standard Hermitian scalar product $(\cdot, \cdot)$ we get

$$|\text{tr}\left(A_1 A_2\right)| = |\text{tr}\left(BA_1B\right)| = \left|\sum_{j=1}^N (BA_1Be_j, e_j)\right| = \left|\sum_{j=1}^N (A_1Be_j, Be_j)\right|$$

$$\leq \ \sum_{j=1}^{N} |A_1| \cdot |Be_j|^2 \ = \ |A_1| \cdot \sum_{j=1}^{N}(B^2 e_j, e_j) \ = \ |A_1| \cdot \operatorname{tr}(A_2).$$

$\square$

Proposition 4.5. *Let M be an n-dimensional compact Riemannian manifold without boundary. For any $x \in M$ and $r > 0$ let $\omega_x(r)$ denote the volume of the geodesic ball about x with radius r. Then there are constants $c_1 > 0$ and $c_2 \in \mathbb{R}$ such that for any $t > 0$ and any $\hbar > 0$ one has*

$$Z_Q(\hbar) \leq c_1 \cdot e^{c_2 \cdot t \hbar^2} \int_M \frac{\operatorname{tr}\left(e^{-tV(x)}\right)}{\omega_x(\sqrt{t\hbar^2})} \, dx. \tag{20}$$

Proof. We apply Lemma 4.3 with $B = t\hbar^2 \nabla^* \nabla$ and $C = t(V + \hbar^2 W)$ and use the notations $k_t^{\nabla^* \nabla}(x,y)$ and $k_t^{\Delta}(x,y)$ for the kernels of the heat operators $e^{-t\nabla^* \nabla}$ and $e^{-t\Delta}$ respectively, where Δ is the Laplace-Beltrami operator acting on functions:

$$
\begin{aligned}
Z_Q(\hbar) \ &\leq \ \operatorname{Tr}\left(e^{-t\hbar^2 \nabla^* \nabla} e^{-t(V + \hbar^2 W)}\right) \\
&= \ \int_M \operatorname{tr}\left(k_{t\hbar^2}^{\nabla^* \nabla}(x,x) e^{-t(V(x) + \hbar^2 W(x))}\right) dx \\
&\overset{(19)}{\leq} \ \int_M \left|k_{t\hbar^2}^{\nabla^* \nabla}(x,x)\right| \cdot \operatorname{tr}\left(e^{-t(V(x) + \hbar^2 W(x))}\right) dx \\
&\leq \ \int_M k_{t\hbar^2}^{\Delta}(x,x) \operatorname{tr}\left(e^{-t(V(x) + \hbar^2 W(x))}\right) dx
\end{aligned}
$$

where for the last inequality we have the Hess-Schrader-Uhlenbrock inequality, i.e. $\left|k_t^{\nabla^* \nabla}(x,y)\right| \leq k_t^{\Delta}(x,y)$ for any $x,y \in M$ and $t > 0$ (see [6]). Applying Lemma 4.3 once more (with $B = tV(x)$ and $C = t\hbar^2 W(x)$), using Lemma 4.4 and choosing a $w_0 \in \mathbb{R}$ with $W \geq w_0$ leads to

$$
\begin{aligned}
Z_Q(\hbar) \ &\leq \ \int_M k_{t\hbar^2}^{\Delta}(x,x) \operatorname{tr}\left(e^{-tV(x)} e^{-t\hbar^2 W(x)}\right) dx \\
&\leq \ \int_M k_{t\hbar^2}^{\Delta}(x,x) \, e^{-t\hbar^2 w_0} \operatorname{tr}\left(e^{-tV(x)}\right) dx. \tag{21}
\end{aligned}
$$

From [11, Thm. 4.6] we get a pointwise estimate for the heat kernel of the Laplace-Beltrami operator: There are constants $c_1, \widetilde{c} > 0$ such that for any $\tau > 0$ and any $x \in M$ one has

$$k_\tau^{\Delta}(x,x) \leq c_1 \cdot \frac{1}{\omega_x(\sqrt{\tau})} \cdot e^{\widetilde{c} \cdot \tau}. \tag{22}$$

Inserting this into (21) and taking $c_2 = \widetilde{c} - w_0$ yields the claim. $\square$

Remark 4.6. The constants c_1, c_2 can be given explicitly: Let $\alpha > 1$, $\delta > 0$ and $n = \dim(M)$, let $\kappa > 0$ with $\operatorname{Ric} \geq -\kappa$ and let $w_0 \in \mathbb{R}$ with $W \geq w_0$. In (22) one can take $c_1 = (1 + \delta)^{n\alpha} \exp\left(\frac{1+\alpha}{\delta}\right)$ and $\widetilde{c} = \frac{\alpha n}{\alpha - 1} \cdot \kappa \cdot \delta$ (compare [11, Thm. 4.6]) and then $c_2 = \widetilde{c} - w_0$.

Given $K \in \mathbb{R}$ and $r \in (0, \frac{\pi}{\sqrt{K}})$ (where we use the convention $\frac{\pi}{\sqrt{K}} = \infty$ for $K \leq 0$) let $v_{K,n}(r)$ denote the volume of a geodesic ball of radius r in the n-dimensional model space of constant curvature K. Recall that this model space is hyperbolic space, Euclidean space, or the sphere with their appropriately scaled standard metrics.

Corollary 4.7. *Let M be an n-dimensional compact Riemannian manifold without boundary, and let $K \in \mathbb{R}$ be an upper bound for the secional curvature of M and let ι denote the injectivity radius of M. Then there are constants $c_2, c_3 \in \mathbb{R}$ such that for any $t, \hbar > 0$ with $t\hbar^2 < \frac{\pi^2}{K}$ and $t\hbar^2 < \iota^2$ we have*

$$\frac{Z_Q(\hbar)}{Z_C(\hbar)} \leq c_3 \cdot e^{c_2 \cdot t\hbar^2} \cdot \frac{v_{0,n}\left(\sqrt{t\hbar^2}\right)}{v_{K,n}\left(\sqrt{t\hbar^2}\right)}.$$

Proof. For $r < \min\{\iota, \frac{\pi}{\sqrt{K}}\}$ the Bishop-Günther Theorem [3, Thm. 3.7] states $\omega_x(r) \geq v_{K,n}(r)$ for all $x \in M$. Inserting this into (20) yields

$$Z_Q(\hbar) \leq c_1 \cdot e^{c_2 \cdot t\hbar^2} \cdot \frac{1}{v_{K,n}\left(\sqrt{t\hbar^2}\right)} \cdot \int_M \operatorname{tr}\left(e^{-tV(x)}\right) dx$$

$$= c_1 \cdot e^{c_2 \cdot t\hbar^2} \cdot \frac{1}{v_{K,n}\left(\sqrt{t\hbar^2}\right)} \cdot (2\sqrt{\pi}t\hbar)^n \cdot Z_C(\hbar)$$

for any $t, \hbar > 0$ with $t\hbar^2 < \frac{\pi^2}{K}$ and $t\hbar^2 < \iota^2$. Putting $c_3 := c_1 \cdot \frac{(2\sqrt{\pi})^n}{v_{0,n}(1)}$ concludes the proof. $\square$

Remark 4.8. Even optimal choices of α and δ yield a constant c_3 which is much larger than 1. Therefore Corollary 4.7 does not even imply half of Corollary 4.2, namely

$$\lim_{\hbar \searrow 0} \frac{Z_Q(\hbar)}{Z_C(\hbar)} \leq 1.$$

We do not know whether Corollary 4.7 holds with $c_3 = 1$.

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